Supplementary Information

Metal ion coordination enhancing quantum efficiency of ligand phosphorescence in a double-stranded helical chain coordination polymer of Pb^{2+} with nicotinic acid

Xiao-Shuo Wu,[a] Yi-Xiong Wang,[b] Shan-Qing Li,[c] Yin Qian,[a] Lu Zhai,*[a] Xiao-Zu Wang,[b] Xiao-Ming Ren*[a,d]

[a] State Key Laboratory of Materials-Oriented Chemical Engineering and College of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 210009, P. R. China

[b] College of Chemical Engineering, Nanjing Tech University, 5 Xinmofan Road, Nanjing 210009, PR China

[c] School of Chemistry and Materials Engineering, Chizhou University, Chizhou, 247000, PR China

[d] State Key Laboratory of Coordination Chemistry, Nanjing University 210093, P. R. China

Fax: 86-25-58139481

Tel: 86-25-58139476

E-mail: zhailu@njtech.edu.cn (LZ); xmren@njtech.edu.cn (XMR)

Contents

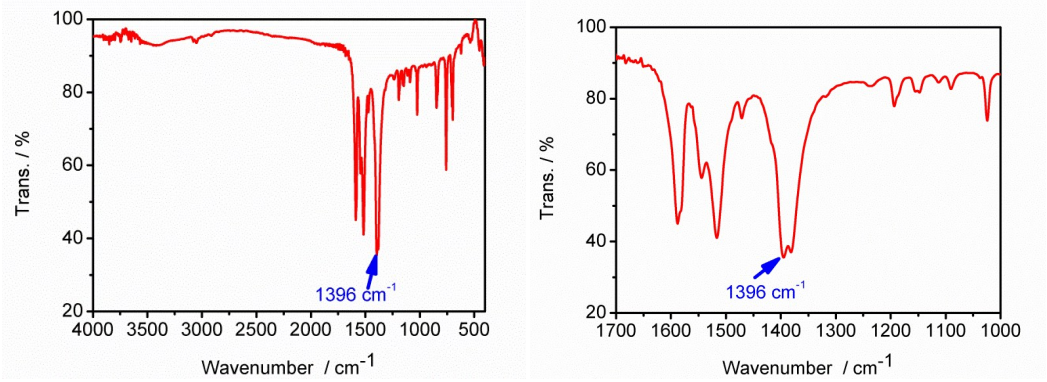


Fig. S1: IR spectrum of **1**.

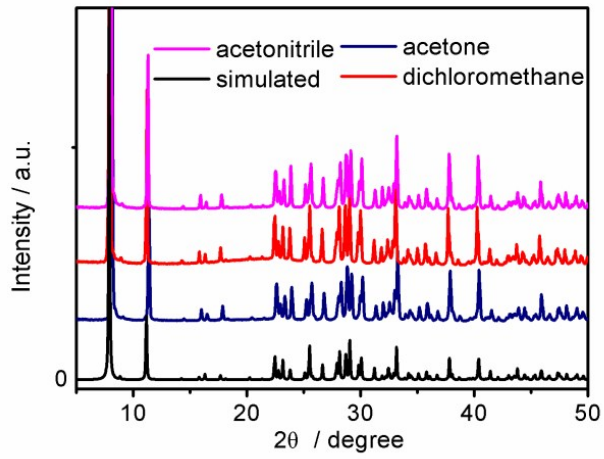


Fig. S2: PXRD patterns of **1** immersed in common organic solvents for 48 hours.

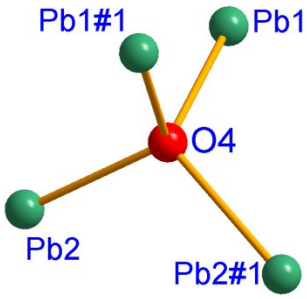


Fig. S3: μ4-oxygen anion connecting four Pb(II) ions, where the symmetric code: #1 = y-1/4, -x+3/4, z-1/4 in **1**.

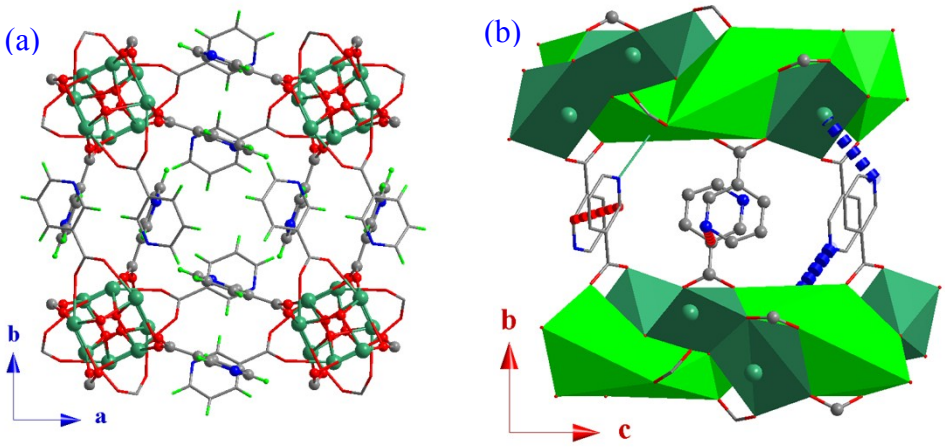


Fig. S4: (a) Arrangement of pyridyl rings between the neighboring 1D double stranded helix chains in **1**, where the 'sticks' mode and the 'balls and sticks' mode represent the nicotinate with N1 and N2, respectively. (b) The dash lines show the shortest interatomic distances where $d_{Pb1\ldots N1}$ = 3.292 Å and $d_{Pb2\ldots N1}$ = 3.551 Å (cyan lines); and $d_{C7\ldots C7}$ = 3.409 Å (centroid-to-centroid distance of 5.739 Å) and $d_{C9\ldots N2}$ = 3.870 Å (centroid-to-centroid distance of 4.092 Å) between the parallel pyridyl rings (red lines).

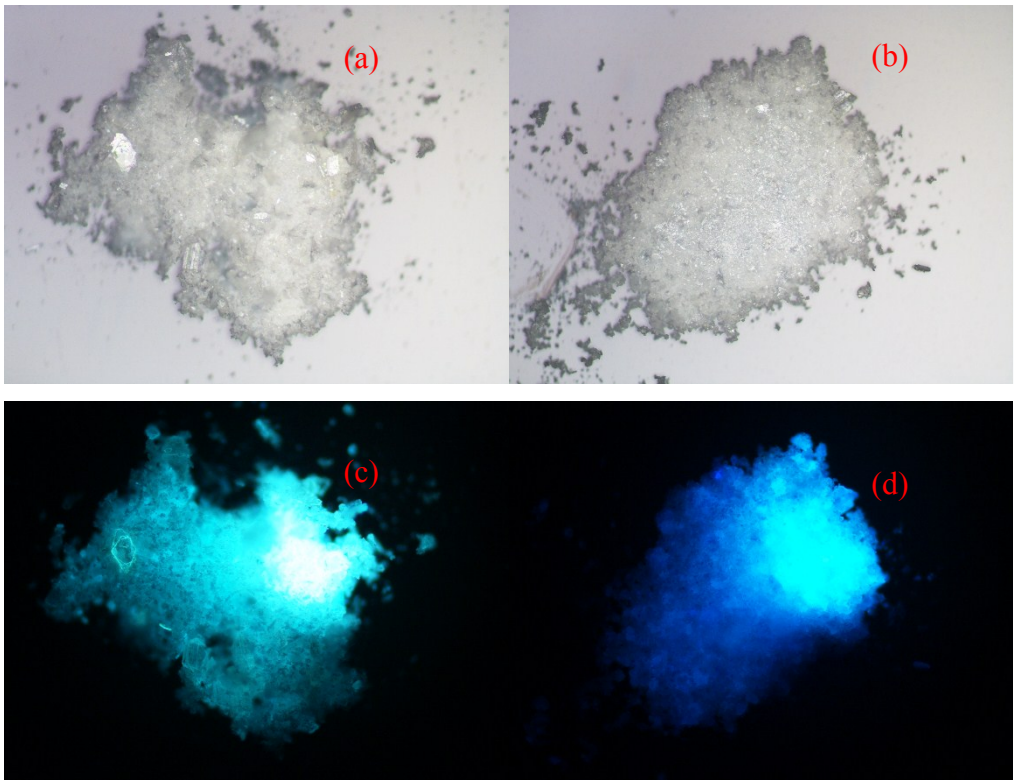


Fig. S5: Images of **1** and nicotinic acid (a, b) under daylight and (c, d) UV light (λ = 330-380 nm).

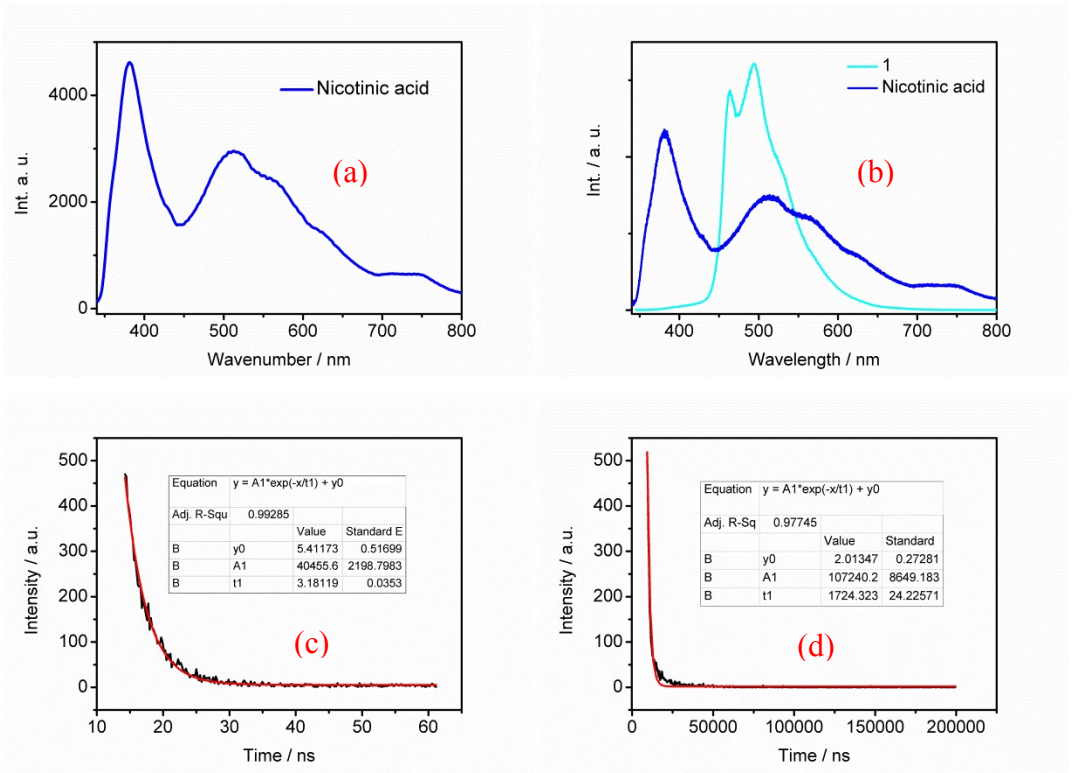


Fig. S6: (a, b) Solid state emission spectra of nicotinic acid and **1** upon the excitation at 325 nm at ambient condition and the luminescence decay curves of nicotinic acid for the emission band with (c) λ_{em} = 380 nm (d) λ_{em} = 510 nm.

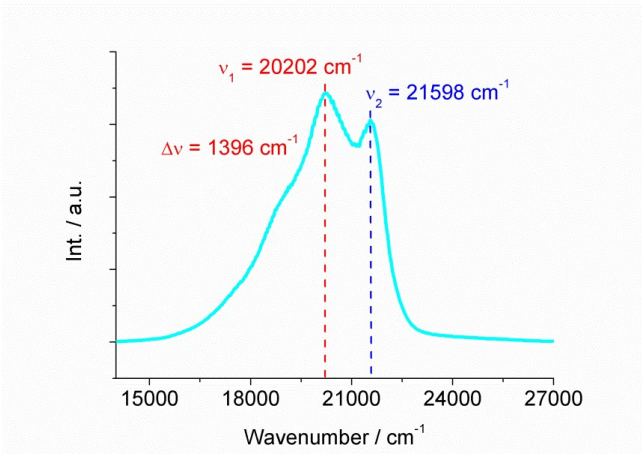


Fig. S7: Solid state emission spectrum of **1** at ambient condition where the horizontal axis is in the form of wavenumber.

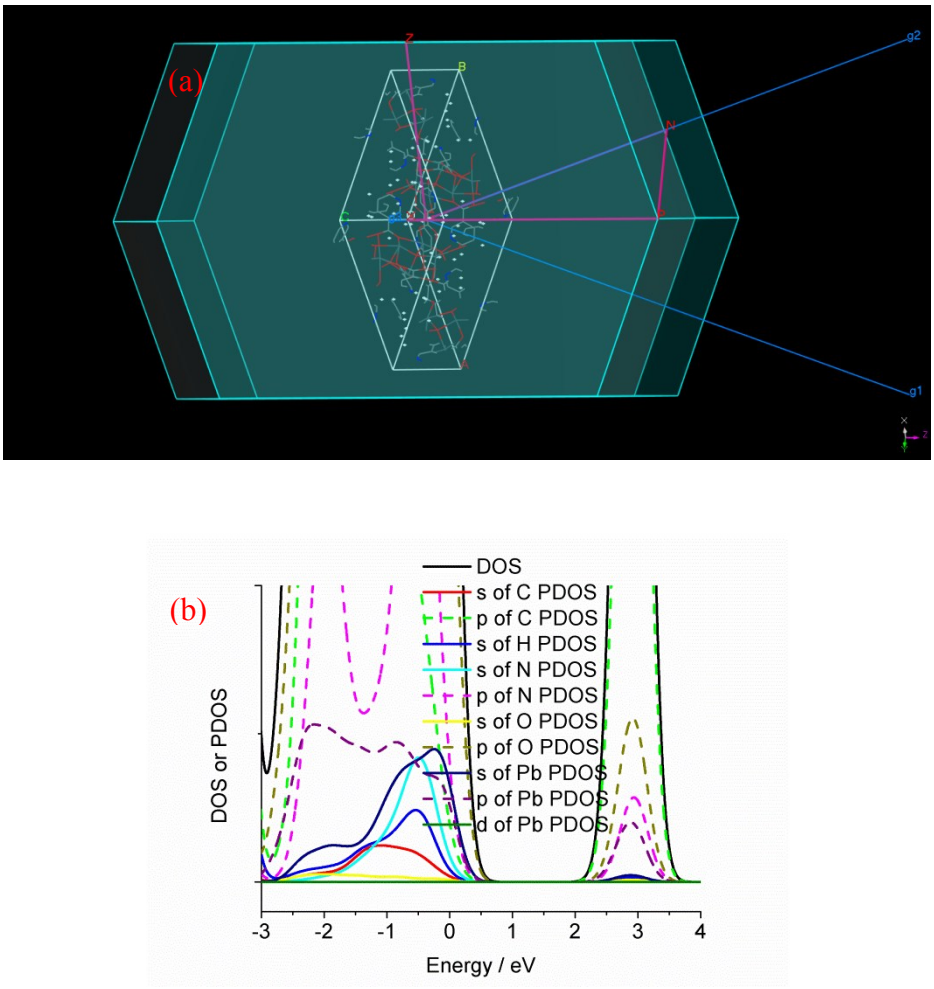


Fig. S8: (a) Brillouin zone (b) Enlarger plots DOS and PDOS of **1**.

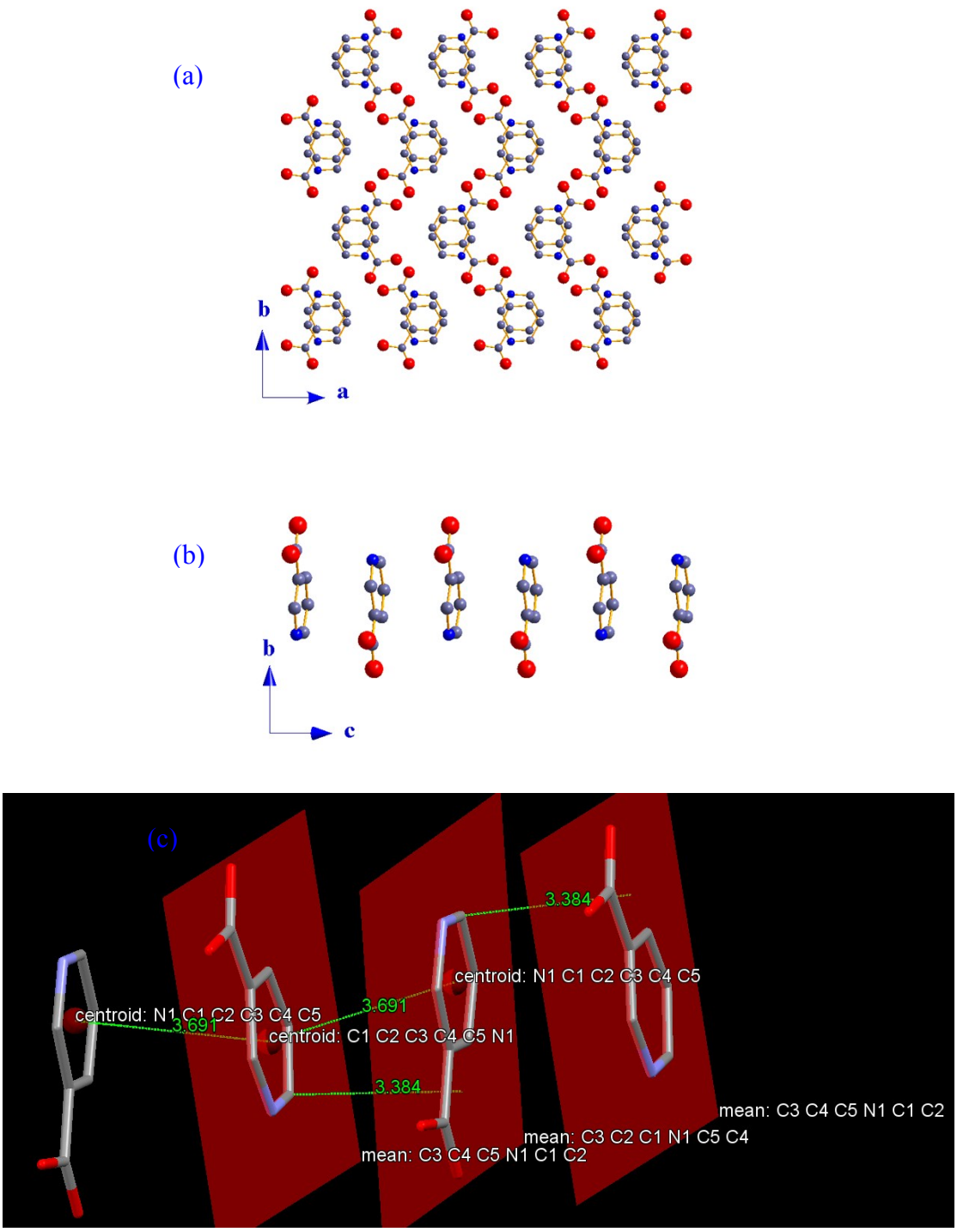
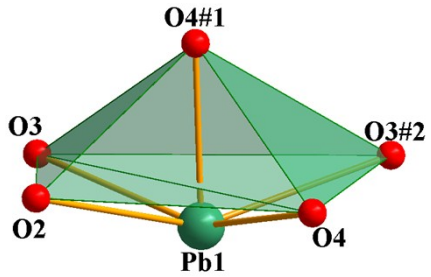
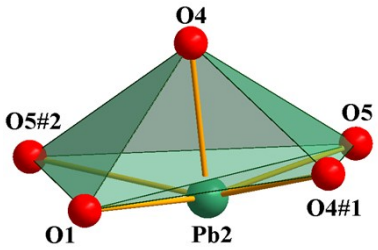


Fig. S9: (a) Packing diagram in the crystal structure of nicotinic acid (b) one π-stacking column (c) illustration of typical distances of centroid-to centroid and the closest atom to mean molecule plane of pyridyl ring.

Table S1: Bond lengths (A) and bond angles (°) in coordination polyhedra of **1**



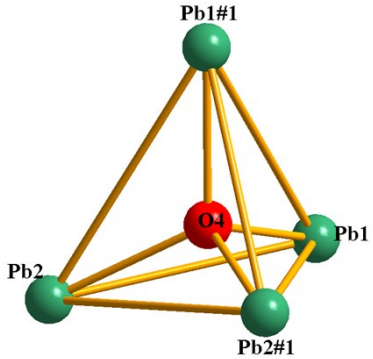
Bond length/Å		Bond angle/°		Bond angle/°	
Pb1-O4	2.311(4)	O4-Pb1-O4#1	77.77(12)	O2-Pb1-O3	68.3(2)
Pb1-O4#1	2.313(5)	O4-Pb1-O2	93.6(2)	O4-Pb1-O3#2	76.30(18)
Pb1-O2	2.485(6)	O4#1-Pb1-O2	74.27(19)	O4#1-Pb1-O3#2	78.03(19)
Pb1-O3	2.716(6)	O4-Pb1-O3	152.00(18)	O2-Pb1-O3#2	152.0(2)
Pb1-O3#2	2.741(6)	O4#1-Pb1-O3	76.77(17)	O3-Pb1-O3#2	109.3(2)



Bond length/Å		Bond angle/°		Bond angle/°	
Pb2-O4	2.231(5)	O4-Pb2-O4#1	78.76(13)	O1-Pb2-O5	164.6(2)
Pb2-O4#1	2.342(4)	O4-Pb2-O1	81.9(2)	O4-Pb2-O5#2	77.08(17)
Pb2-O1	2.482(7)	O4#1-Pb2-O1	92.1(2)	O4#1-Pb2-O5#2	151.21(17)
Pb2-O5	2.683(6)	O4-Pb2-O5	85.35(19)	O1-Pb2-O5#2	69.3(2)
Pb2-O5#2	2.757(6)	O4#1-Pb2-O5	76.88(17)	O5-Pb2-O5#2	116.2(2)

Symmetry transformations used to generate equivalent atoms: #1 = y-1/4, -x+3/4, z-1/4; #2 = y+3/4, x+1/4, z+1/4

Table S2 Bond lengths (A) and bond angles (°) in Pb_4O cluster of **1**



Bond length/Å		Bond angle/°	
Pb1...Pb2	3.4831(1)	Pb1-O4-Pb2	96.893
Pb1...Pb1#1	3.8031(2)	Pb1-O4-Pb1#1	110.717
Pb1...Pb2#1	3.8747(1)	Pb1-O4-Pb2#1	116.999
Pb2...Pb1#1	4.0264(3)	Pb2-O4-Pb1#1	119.879
Pb2...Pb2#1	3.8209(2)	Pb2-O4-Pb2#1	113.294

Symmetry transformations used to generate equivalent atoms: #1 y-1/4, -x+3/4, z-1/4